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CFD Modeling For Urban Air Quality Studies

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3.3 CFD MODELING FOR URBAN AIR QUALITY STUDIES

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1. INTRODUCTION

The computational fluid dynamics (CFD) approach has been increasingly applied to many atmospheric applications, including flow over buildings and complex terrain, and dispersion of hazardous releases. However there has been much less activity on the coupling of CFD with atmospheric chemistry. Most of the atmospheric chemistry applications have been focused on the modeling of chemistry on larger spatial scales, such as global or urban airshed scale. However, the increased attentions to terrorism threats have stimulated the need of much more detailed simulations involving chemical releases within urban areas. This motivated us to develop a new CFD/coupled-chemistry capability as part of our modeling effort.

The model we have developed is based on the FEM3MP CFD model with a coupled chemistry submodel, which uses SMVGEAR II as the chemistry solver. The CFD/Chemistry model has initially been applied to chemically reactive releases around buildings. These local-scale flow computations are typically based on domain sizes of one to a few kilometers square with highly graded meshes to resolve the complicated flows associated with building wakes interactions. A selection of these simulations will be presented at this conference.

More recently, we have explored the use of the CFD approach to study air quality within urban areas. It is clear that some compromises in grid resolution have to be made due to the larger domain sizes that are of interest. However, even with the somewhat coarser grid sizes, the typical grid resolutions are approximately an order of magnitude finer than that used in mesoscale simulations. With the finer resolution, CFD calculations can resolve terrain and can even model building effects with higher fidelity. This should lead to more accurate predictions of wind fields and dispersion patterns.

Several challenges nevertheless must still be overcome. For example, the limited area representation requires boundary conditions that must be driven from large-scale forecasts. These boundary conditions include not only the usual meteorological fields, but also the chemical pollutants that advect into the domain from sources outside of the computational zone. Another issue that needs to be addressed is that the inventory of sources within the domain should be consistent with the finer grid resolution. Due to the somewhat unreliable estimates of release rates from power plants and unpredictable meteorological conditions, it is often difficult to obtain very precise spatial inventories of source terms.

In the air quality study, we have focused on the high ozone level episode that occurred in the Livermore Valley on July 31, 2000. Some preliminary simulations of the July 31 episode using two widely used mesoscale forecast models and an urban airshed model have not been able to recreate the occurrence of high ozone condition in the appropriate locations within the Valley. In this meeting, we will present some results of our simulations of wind and dispersion patterns for this particular scenario. The results are based on using relatively fine grid resolutions and concomitantly better representation of the terrain upwind of the Livermore Valley. Initial results show that the wind patterns are highly influenced by local topography that contributed to the channeling of the northerly mean flow down the valley towards the Livermore Valley.

2. THE FEM3CHEM MODEL

The numerical model used in this study (FEM3CHEM) is an extension of a finite-element-based CFD model used to simulate building-scale flows. The basic flow model solves the time-dependent, incompressible Navier-Stokes equations using graded and distorted elements to represent the geometric complexities associated with buildings and other urban configurations. The coding structure of the model is based on an object-oriented approach with message passing for achieving parallelization. For flexibility, the model contains a number of different RANS (Reynolds Averaged Navier-Stokes) turbulence closures; a K-theory model, buoyancy-extended k-epsilon, an advanced nonlinear eddy viscosity model, and a Large-Eddy Simulation (LES) model. The model also

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contains a number of physics submodels for simulating flow and dispersion within urban areas (Lee, et al., 2001)

In FEM3CHEM, we have enhanced the flow model with a chemistry component based on the SMVGEAR chemistry solver (Jacobsen,1994). The front end of the chemistry model is based on a unique interface developed in LLNL's IMPACT model (Atherton, et al., 1998) wherein selected chemical mechanisms are automatically inserted into the chemistry module. The flow/chemistry coupling is achieved via a fractional time-splitting procedure in which the flow and chemistry timesteps are performed alternatively. Fixed timesteps are used for advancing the flow physics but chemistry timesteps are variable and interpolated, if necessary, to coincide with timesteps for the CFD component.

3. SIMULATIONS OF RELEASES IN THE LIVERMORE VALLEY

The simulation of interest is motivated by the air quality problems that exist within the Livermore Valley east of San Francisco. Over the past decade, there has been increasing concern that Livermore and its neighboring cities have reported ozone levels, which exceeded the EPA standards over the allowable number of days during the summer season. There is some conjecture that the air quality problems were caused by releases from the oil refineries at Martinez, about 20 miles northwest of Livermore, and vehicular emissions from Interstate 680 corridor which cuts across the Valley in a north-south direction. The Bay Area Air Quality Management District has conducted modeling studies of the July 31, 2000 incident when the ozone levels were observed to be particularly high. However, the studies thus far did not appear to generate wind patterns that clearly supported the transport of the contaminants towards the Livermore area. Part of the reason may be due to the coarseness of the 4 km grid spacing employed in the study that did not have the necessary resolution to resolve the topographical features of the local terrain. Recent simulations have started to use 1 km grid cells in order to achieve better resolution of the local terrain.

Our CFD simulations are based on a domain size of 70 km x 80 km with a grid resolution of 500 m and a height of 2 km. Within this area, this grid size is capable of resolving many of the coastal hills and, in particular, the highest mountain Mount Diablo which rises to a height of over 1.1 km above sea level (fig. 1). In order to simplify the source representations, we have assumed a uniform *elevated* source of approximately 6 sq km above Martinez and a constant flux *ground* source along Interstate 680. The tracers released are assumed to be *non-reacting* since the purpose of this study is to attempt to simulate the dispersion patterns carried downwind from the sources. A steady-state mean wind of 8 m/s approaching from the northwest (315°) was used as the initial condition. At the upwind boundaries, the mean wind was modeled by assuming a constant counterclockwise rotation from northwest (315°) to west (270°) during the period of 1 hour. This flow pattern roughly resembles the wind station observations recorded on the afternoon of July 31, 2000 when the ozone levels were at a maximum. The simulations were performed for 1 hour after the initial releases.

Fig. 2 shows the initial condition for the simulation as depicted by the northwest mean flow and the elevated release over the Martinez area and the ground release along Interstate 680. As the mean wind shifts from the northwest to the westerly direction, the plume was transported toward the east to the Livermore area.

The development of the wind field and dispersion patterns (depicted here as isosurface plots) at 200 secs and 1 hr are shown in figs. 3 and 4, respectively. After 1 hr the mean wind has shift completely to the west and the plume has broaden significantly with a portion of the I-680 plume covering the western part of Livermore. It is clear that the 1 hr duration of the simulation is probably a bit short and did not allow the Martinez cloud to reach the Livermore area. Nevertheless, the simulated wind pattern depicted roughly the correct trend, which, in time, will contribute to the air quality problems in the Livermore Valley.

4. ACKNOWLEDGEMENT

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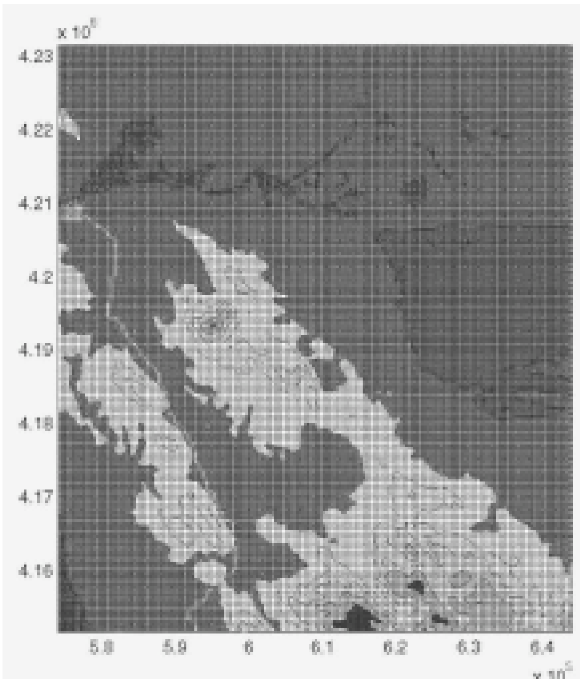

Fig.1: 500 m resolution terrain map for the modeled domain showing the Interstate 680 highway.

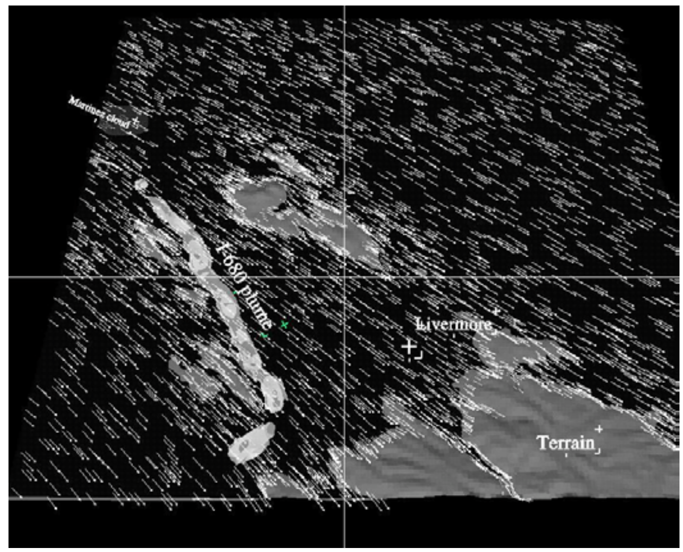

Fig.3: Dispersion patterns for Martinez (elevated) and I-680 (surface) releases at 200 secs.